CRN 109-97-7 CMF C4 H5 N



IT 7647-10-1, Palladium dichloride

RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalysts containing polypyrrole and mol. sieves and, for oxidation of
 cyclohexane)

RN 7647-10-1 HCAPLUS

CN Palladium chloride (PdCl2) (6CI, 8CI, 9CI) (CA INDEX NAME)

Cl-Pd-Cl

IT 14172-90-8 16591-56-3

RL: CAT (Catalyst use); USES (Uses) (catalysts containing, for oxidation of cyclohexane)

RN 14172-90-8 HCAPLUS

RN 16591-56-3 HCAPLUS

CN Iron, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX
NAME)

IT 108-93-0P, Cyclohexanol, preparation 108-94-1P,
 Cyclohexanone, preparation 124-04-9P, Adipic acid, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (improved synthesis of, by oxidation of cyclohexane)
RN 108-93-0 HCAPLUS
CN Cyclohexanol (8CI, 9CI) (CA INDEX NAME)



RN 108-94-1 HCAPLUS CN Cyclohexanone (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 124-04-9 HCAPLUS CN Hexanedioic acid (9CI) (CA INDEX NAME)

 $HO_2C-(CH_2)_4-CO_2H$

67-64-1, Acetone, uses ΙT

RL: USES (Uses)

(solvent, for oxidation of cyclohexane)

RN 67-64-1 HCAPLUS

CN 2-Propanone (9CI) (CA INDEX NAME)

0 H3C-C-CH3

L43 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:228526 HCAPLUS

DOCUMENT NUMBER:

114:228526

TITLE:

Preparation of secondary-butyltoluene hydroperoxide

INVENTOR(S):

Ono, Hiroyasu; Yorozu, Kiyotaka

PATENT ASSIGNEE(S):

Mitsui Petrochemical Industries, Ltd., Japan Jpn. Kokai Tokkyo Koho, 4 pp.

SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

1

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

-----_____ JP 03011058 A2 19910118 JP 1989-146109 19890608 <--

PRIORITY APPLN. INFO.:

JP 1989-146109 19890608 <--

GΙ

OTHER SOURCE(S): CASREACT 114:228526; MARPAT 114:228526

AB The title compound is prepared in high selectivity to tertiary hydroperoxide (I) by treatment of EtCHMeC6H4Me (II) with O-containing gas in the presence of ≥1 complex of alkaline earth metal or transition metal with tetraphenylporphyrins. A mixture of II, an aqueous Na2CO3 solution, and porphyrin-Mg2+ complex III was heated under bubbling with air to 120° and I was added to initiate the reaction, concentration of I in the reaction product after 3 h was 12.0%, vs. 1.0% for a control without addition of III.

TT 14172-91-9 14172-92-0 14640-21-2 14705-63-6 16456-81-8

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for oxidation of sec-butyltoluene, tertiary hydroperoxide from)

RN 14172-91-9 HCAPLUS

CN Copper, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX
NAME)

III

RN 14172-92-0 HCAPLUS

CN Nickel, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 14640-21-2 HCAPLUS CN Magnesium, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)kN21,kN22,kN23,kN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 14705-63-6 HCAPLUS CN Vanadium, $oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-\kappa N21,\kappa N22,\kappa N23,\kappa N24]-$, (SP-5-12)- (9CI) (CA INDEX NAME)

RN 16456-81-8 HCAPLUS CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-KN21,KN22,KN23,KN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



D1-Me

$$\begin{array}{c} \text{D1} \\ | \\ \text{Me-CH-Et} \end{array}$$

ΙT 113588-16-2P, 2-Tolyl-2-hydroperoxybutane

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by catalytic oxidation of sec-butyltoluene)

RN 113588-16-2 HCAPLUS

CN Hydroperoxide, 1-methyl-1-(methylphenyl)propyl (9CI) (CA INDEX NAME)



D1-Me

L43 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:188007 HCAPLUS

DOCUMENT NUMBER:

114:188007

TITLE:

Production of detergent range alcohols and ketones

from alkanes using porphyrin catalysts

INVENTOR(S):

Sanderson, John R.; Marquis, Edward T.; Payton, Howard

F.

PATENT ASSIGNEE(S):

Texaco Chemical Co., USA

SOURCE:

U.S., 11 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------|---------|----------------------|----------------------------------|--------------------------|
| US 4978799 EP 426290 | A A2 | 19901218 19910508 | US 1989-428812 EP 1990-310155 | 19891030 < 19900917 < |
| EP 426290 | A3 | 19910925 | EF 1990-310133 | 19900917 < |
| R: DE, FR, | • | | | |
| JP 03169831 | A2 | 19910723 | JP 1990-290985 | 19901030 < |
| PRIORITY APPLN. INFO | . : | | US 1989-428701 | 19891030 < |
| | | | US 1989-428703 | 19891030 < |
| | | | US 1989-428812 | 19891030 < |

The reaction of C10-18 alkanes with a hydroperoxide, especially tert-BuOOH or AB cumene hydroperoxide (I), in the presence of a transition metal (especially Fe, Mn, or Co) porphyrin catalyst gives alcs. and ketones with minimal formation of byproducts. A mixture of dodecane 50.0, chloroferric phthalocyanine 0.10, and imidazole 0.07 g was treated slowly at 30° with 80% I to give 5.02% dodecanones and 1.42% dodecanols.

132-16-1, Ferrous phthalocyanine 142-71-2, Cupric ITacetate 147-14-8, Cupric phthalocyanine 288-32-4, Imidazole, uses and miscellaneous 536-80-1, Iodosylbenzene 1643-19-2, Tetrabutylammonium bromide 4328-13-6,
Tetrahexylammonium bromide 7601-89-0, Sodium perchlorate
12030-88-5, Potassium superoxide 12676-27-6
13395-16-9, Cupric acetylacetonate 14172-90-8
14285-56-4, Chloroferric phthalocyanine 16456-81-8
58356-65-3 60385-96-8
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for oxidation of alkanes to alcs. and ketones)
RN 132-16-1 HCAPLUS
CN Iron, [29H,31H-phthalocyaninato(2-)-kN29,kN30,kN31,kapp a.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 142-71-2 HCAPLUS CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)

●1/2 Cu(II)

RN 147-14-8 HCAPLUS CN Copper, [29H, 31H-phthalocyaninato(2-)-κN29,κN30,κN31,.ka ppa.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A



288-32-4 HCAPLUS RN1H-Imidazole (9CI) (CA INDEX NAME) CN



RN

536-80-1 HCAPLUS Benzene, iodosyl- (9CI) (CA INDEX NAME) CN

o = I - Ph

1643-19-2 HCAPLUS RN

1-Butanaminium, N,N,N-tributyl-, bromide (9CI) (CA INDEX NAME) CN

● Br-

4328-13-6 HCAPLUS CN 1-Hexanaminium, N,N,N-trihexyl-, bromide (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{(CH}_2)\,5^{-}\,\text{Me} \\ | \\ | \\ \text{Me}^{-}\,\,\text{(CH}_2)\,5^{-}\,\text{N}^{+}\,\,\text{(CH}_2)\,5^{-}\,\text{Me} \\ | \\ | \\ \text{(CH}_2)\,5^{-}\,\text{Me} \end{array}$$

RN 7601-89-0 HCAPLUS Perchloric acid, sodium salt (8CI, 9CI) (CA INDEX NAME) CN

12030-88-5 HCAPLUS RN Potassium superoxide (K(O2)) (9CI) (CA INDEX NAME) CN

+ K- O=O

RN

12676-27-6 HCAPLUS Boric acid, lithium salt (9CI) (CA INDEX NAME) CN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 13395-16-9 HCAPLUS

Copper, bis $(2, 4\text{-pentanedionato-}\kappa O, \kappa O')$ -, (SP-4-1)- (9CI) (CA CN INDEX NAME)

RN 14172-90-8 HCAPLUS CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-KN21,KN22,KN23,KN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 14285-56-4 HCAPLUS CN Iron, chloro[29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31, κ N32]-, (SP-5-12)- (9CI) (CA INDEX NAME)

RN 16456-81-8 HCAPLUS CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

RN 58356-65-3 HCAPLUS CN Manganese, (acetato- κ O)[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)- κ N21, κ N22, κ N23, κ N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

RN 60385-96-8 HCAPLUS CN Cuprate(1-), [29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N3 1, κ N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)

27342-88-7P, Dodecanol 35655-31-3P, Dodecanone ΙT RL: PREP (Preparation) (manufacture of, from dodecane, catalysts for) RN 27342-88-7 HCAPLUS Dodecanol (8CI, 9CI) (CA INDEX NAME) CN $Me^{-(CH_2)}10^{-Me}$ D1-OH 35655-31-3 HCAPLUS RN Dodecanone (9CI) (CA INDEX NAME) CN $Me^- (CH_2)_{10}^- Me$ D2== 0 ΙT 75-91-2, tert-Butyl hydroperoxide 80-15-9, Cumene hydroperoxide RL: RCT (Reactant); RACT (Reactant or reagent) (oxidation by, of alkanes to alcs. and ketones) 75-91-2 HCAPLUS RN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME) CN HO-O-Bu-t 80-15-9 HCAPLUS RN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME) CN O-OH Me-C-MePh ΙT 112-40-3, Dodecane RL: RCT (Reactant); RACT (Reactant or reagent) (oxidation of, to alcs. and ketones, catalysts for) RN 112-40-3 HCAPLUS Dodecane (8CI, 9CI) (CA INDEX NAME) CN

 $Me^-(CH_2)_{10}-Me$

L43 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1990:118456 HCAPLUS

DOCUMENT NUMBER:

112:118456

TITLE:

Method of preparing substituted cyclic carboxylic acids by oxidation of cyclic hydrocarbons with air or

oxygen using metal complex catalysts

INVENTOR(S):

Svensson, Nils A.

PATENT ASSIGNEE(S):

Nobel Chemicals AB, Swed. U.S., 3 pp.

SOURCE:

DOCUMENT TYPE:

CODEN: USXXAM

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------|--------|----------|-----------------|------------|
| | | | | |
| US 4866204 | A | 19890912 | US 1988-156036 | 19880216 < |
| SE 8700657 | A | 19880819 | SE 1987-657 | 19870218 < |
| PRIORITY APPLN. | INFO.: | | SE 1987-657 | 19870218 < |

Substituted cyclic carboxylic acids, specifically benzoic and phthalic acids, are prepared by oxidation of corresponding cyclic hydrocarbons with air or O in the liquid phase in an organic solvent under alkaline conditions using metal complex catalysts. The catalysts are Fe, Ni, Mn, or V tetraphenylporphines, or Ni, Cu, Co, Mn, Cr, or Ti phthalocyanines or acetylacetonates, or their mixts. Thus, air was passed forcefully into a mixture of 100 mL MeOH, 34.0 g KOH, 13.7 g o-nitrotoluene, and 10 mg freshly prepared Fe tetraphenylporphine chloride at 25° for 18 h to give o-nitrobenzoic acid in 95% yield.

147-14-8, Copper phthalocyanine 3264-82-2, Nickel TT acetylacetonate 3317-67-7, Cobalt phthalocyanine 13395-16-9, Copper acetylacetonate 14024-48-7 14055-02-8 14172-92-0, Nickel tetraphenylporphine 14284-89-0, Manganese acetylacetonate 14284-96-9 14285-60-0, Chromium phthalocyanine 14325-24-7, Manganese phthalocyanine 14705-63-6 16591-56-3, Iron tetraphenylporphine 21679-31-2, Chromium acetylacetonate

31004-82-7, Manganese tetraphenylporphine 52324-93-3,

Titanium phthalocyanine 125491-21-6

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for oxidation of cyclic hydrocarbons to cyclic carboxylic acids)

147-14-8 HCAPLUS RN

Copper, [29H, 31H-phthalocyaninato(2-)-κN29,κN30,κN31,.ka CN ppa.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 3264-82-2 HCAPLUS

CN Nickel, bis(2,4-pentanedionato-κ0,κ0')-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 3317-67-7 HCAPLUS

CN Cobalt, [29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31,.ka ppa.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 13395-16-9 HCAPLUS
CN Copper, bis(2,4-pentanedionato-κO,κO')-, (SP-4-1)- (9CI) (CA INDEX NAME)

Me Me Me
$$Cu^{2+}$$
 CH Me Me Me Me

RN 14024-48-7 HCAPLUS Cobalt, bis(2,4-pentanedionato- κ O, κ O')-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 14055-02-8 HCAPLUS CN Nickel, [29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,.ka ppa.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)